CONSTITUTIVE MODELS TO DESCRIBE THE RESPONSE OF MATERIALS FOR HIGH TEMPERATURE OPERATING CONDITIONS

K. R . RAJAGOPAL

DEPARTMENT OF MECHANICAL ENGINEERING

TEXAS A&M UNIVERSITY, COLLEGE STATION, TX 77804

TEL: 979 862 4552, FAX: 979 862 3989, EMAIL: KRAJAGOPAL@MENGR.TAMU.EDU

I. J. RAO

DEPARTMENT OF MECHANICAL ENGINEERING

NEW JERSEY INSTITUTE OF TECHNOLOGY, NEWARK, NJ 07102

TEL: 973 596 5601, FAX: 973 642 4282, EMAIL: RAOI@NJIT.EDU

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OBJECTIVES:

1. Develop a robust thermodynamic framework that can describe the response of the class of materials that are being fashioned, connecting the microstructure to the continuum level response.
2. Develop computational tools, through user defined subroutines, to utilize the models developed in the comprehensive finite element software ABAQUS

ACCOMPLISHMENTS TO DATE:

The development of constitutive models that can predict the behavior of materials, specifically metals, at high temperature requires a good understanding of the physical mechanisms that are particularly relevant at high temperatures that lead to behavior such as creep. This behavior then has to be translated into constitutive equations that can be used with the primary equations of mechanics to solve relevant boundary value problems. To model creep in super alloys, we have developed constitutive models within a thermodynamic setting. This thermodynamic framework was developed specifically to handle inelastic materials such as these.

The changes in the microstructure during the process are captured by the fact that the natural configuration of the body, namely the configuration that the body would attain on the removal of the external stimuli, evolves. This evolution is determined by the tendency of the body to undergo a process that maximizes the rate of dissipation. For the problems under consideration it is sufficient to assume that the elastic response is linearly elastic with cubic symmetry (it is possible to easily incorporate other types of symmetries). A form for the inelastic stored energy (the energy that is trapped within the dislocation networks) is introduced based on simple ideas related to the motion of the dislocations. The rate of dissipation is assumed to be proportional to the density of mobile dislocations and another term that takes into account the damage accumulation due to creep.

A User Material Subroutine (UMAT) has been developed so that we can use the commercial software ABAQUS to solve boundary value problems in realistic and relevant geometries. Since the model is highly non-linear it has to be solved sequentially by linearizing the nonlinear problem and iterating towards a solution. This was done by implementing the Jacobian, or tangent stiffness matrix into the subroutine for the specific model developed. The Jacobian developed here is the elasticity matrix for a face centered cubic system. The resulting non-linear equations are then solved using a Newton Raphson method and time integration is carried out using an implicit scheme. This UMAT has been tested for a variety of different cases and the results have been compared with earlier computations as well as against experimental data. These validations tests have been completed successfully.

FUTURE WORK:

1. Develop an optimization program for the choices for the stored energy, rate of entropy production etc. (which in turn imply how the material ought to be engineered) based on a set of desired response characteristics that are used as the benchmark. This interactive optimization scheme will connect the models with the desired outcomes using the ABAQUS software, whereby the models can be systematically varied and their efficacy tested with respect to a desired response.

CONFERENCE PRESENTATIONS and PUBLICATIONS

None

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None

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